([(2-Amino-2-carboxyethyl)sulfanyl]methyl)cystei

Inchi: InChI=1S/C7H14N2O4S2/c8-4(6(10)11)1-14-3-15-2-5(9)7(12)13/h4-5H,1-3,8-9H2,(H,10,
InchiKey: JMQMNWIBUCGUDO-UHFFFAOYSA-N
Formula: C7H14N2O4S2
SMILES: [NH3+]C(CSCSCC([NH3+])C(=O)[O-])C(=O)[O-]
Mol. weight [g/mol]: 254.33

Physical Properties

Property code	Value	Unit	Source
log10ws	0.23		Crippen Method
logp	-4.869		Crippen Method
mcvol	177.030	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005774&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume